

Supplementary Material

Synthesis of a β -isoindigo-linked 1*H*-3-benzazepine-modified aza-boron dipyrromethene dimer

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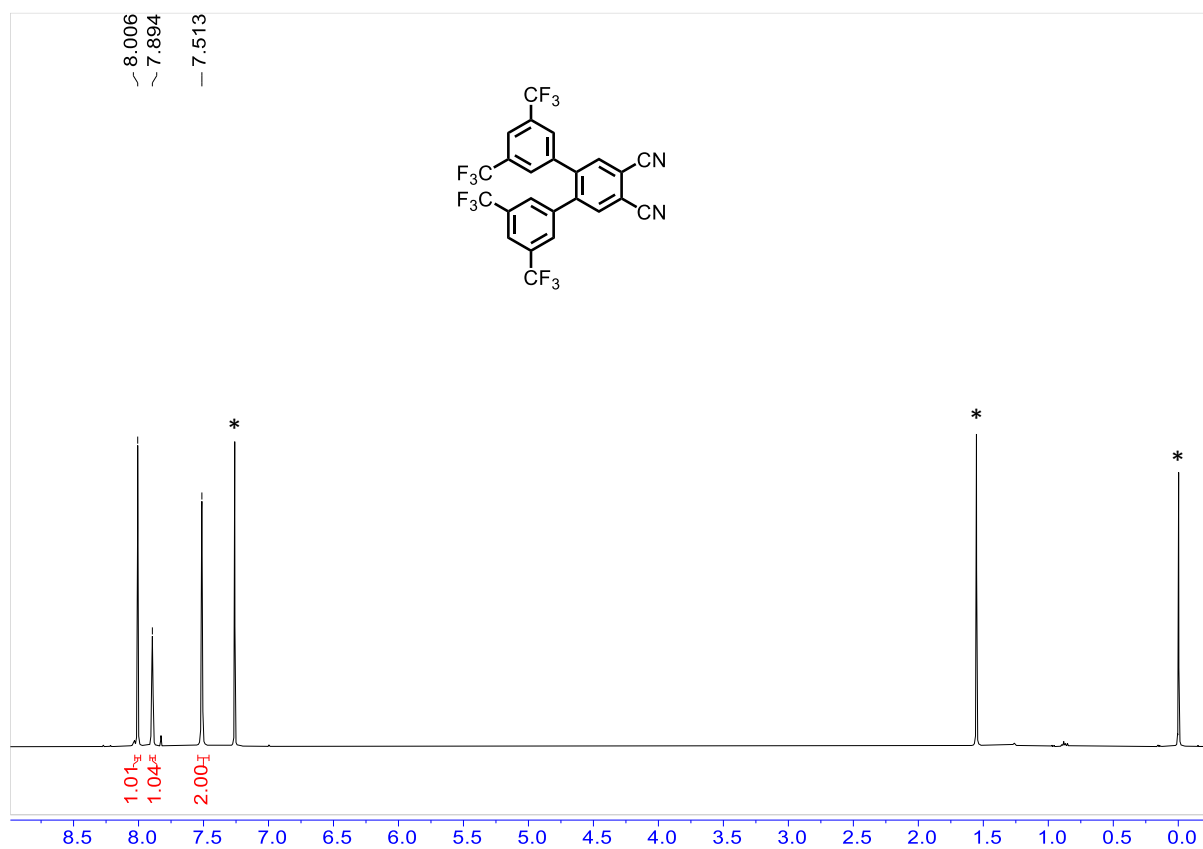


Figure S1. ¹H NMR spectrum of **3** in CDCl₃ (400 MHz). The signals due to the residual non-deuterated solvent, residual water, and SiMe₄ are marked with an asterisk.

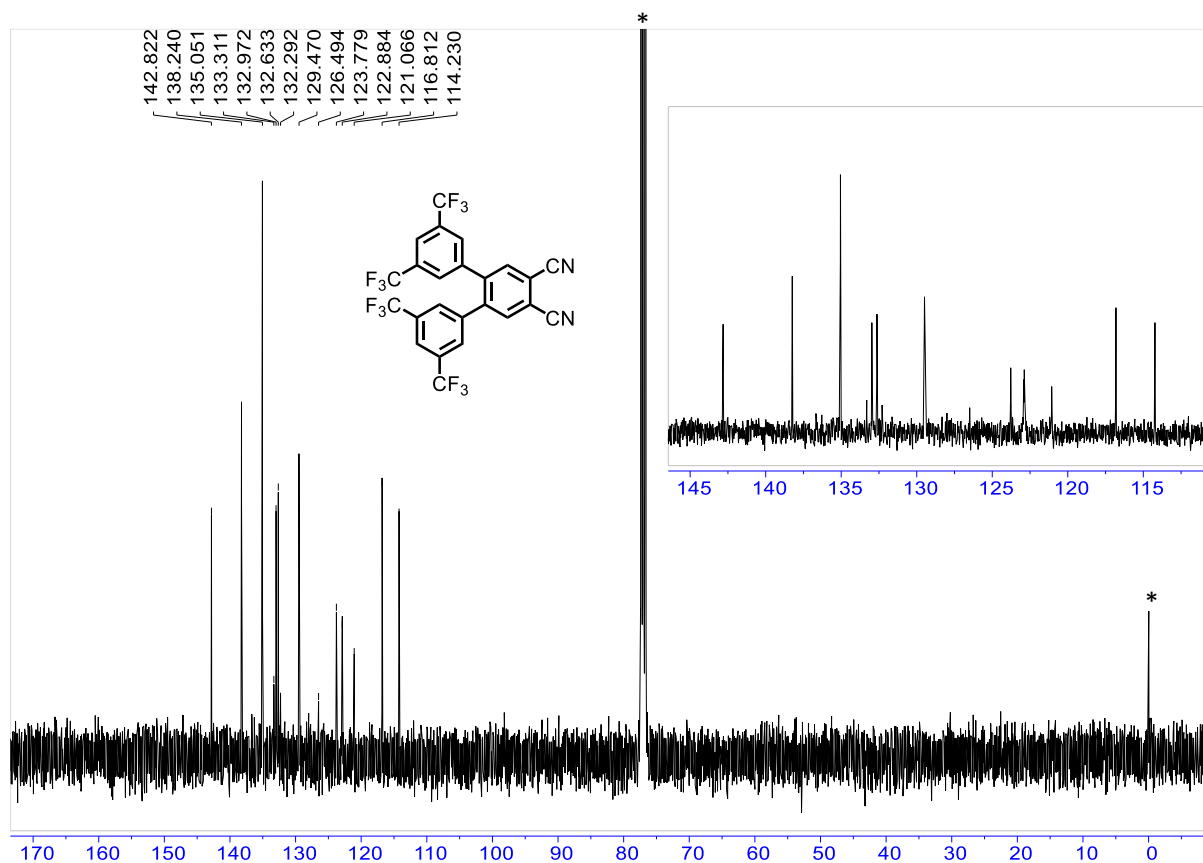


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** in CDCl_3 (100.6 MHz). The signals due to the solvent and SiMe_4 are marked with an asterisk.

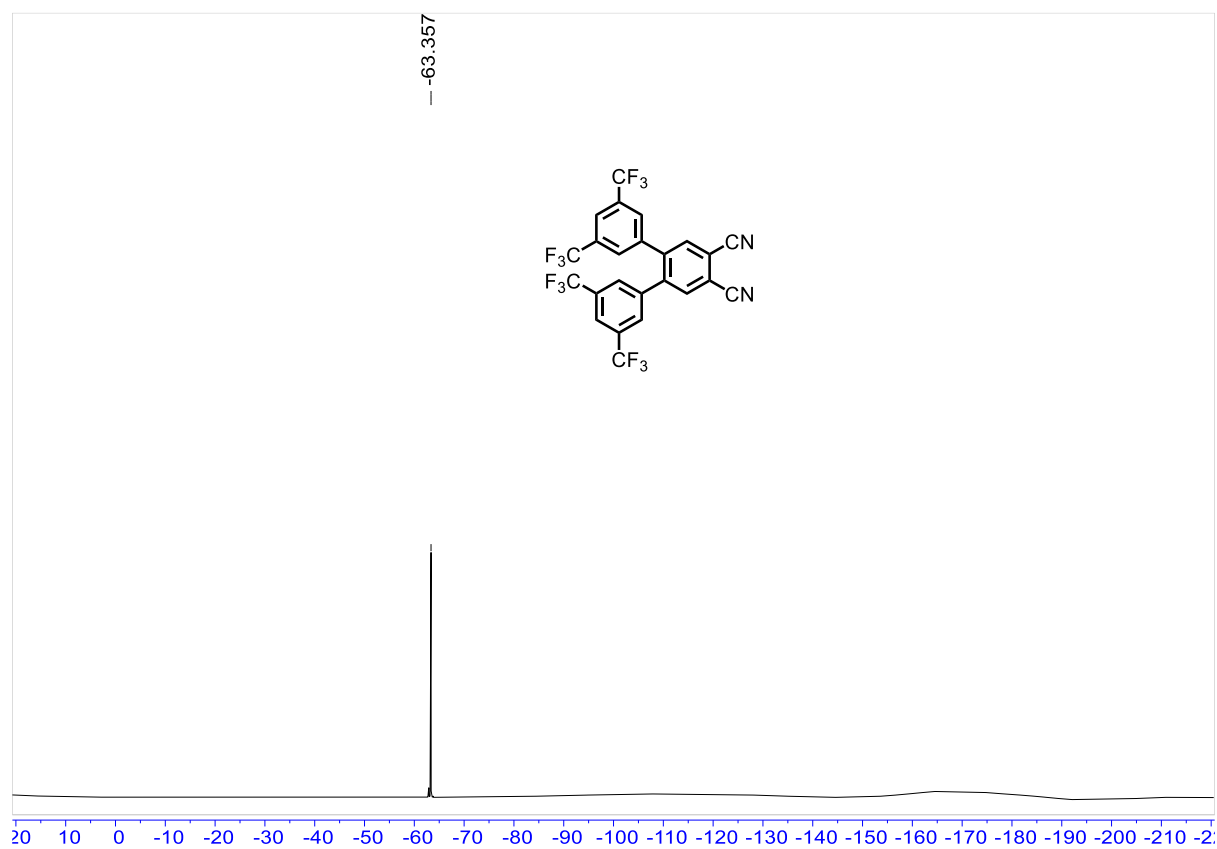


Figure S3. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **3** in CDCl_3 (470.4 MHz).

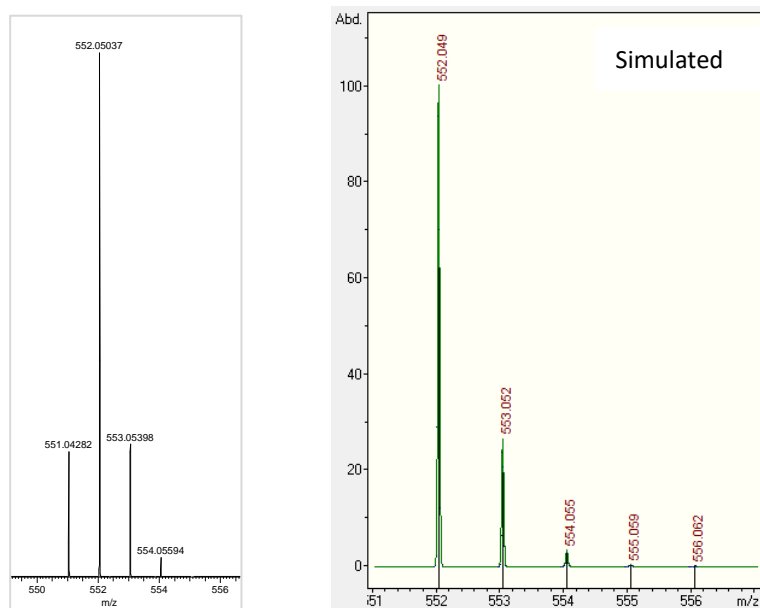
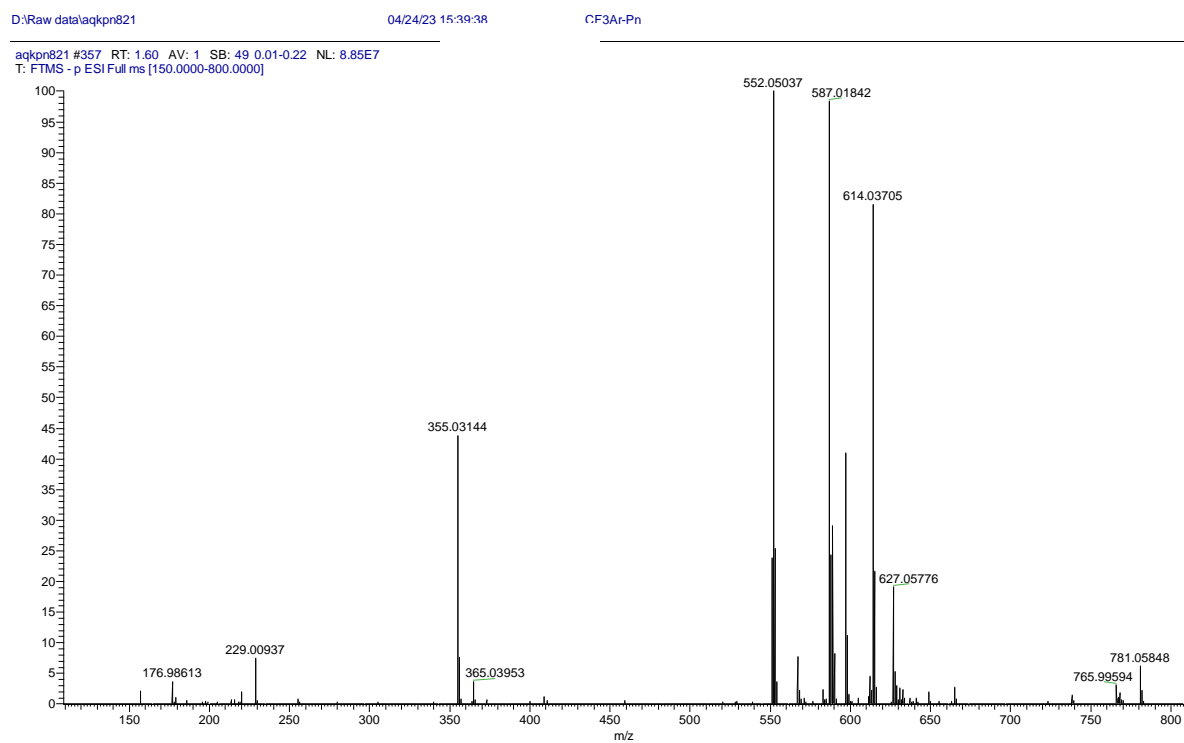


Figure S4. ESI mass spectrum of **3**. The experimental and simulated isotopic patterns of the molecule ion signal are given in the lower part.

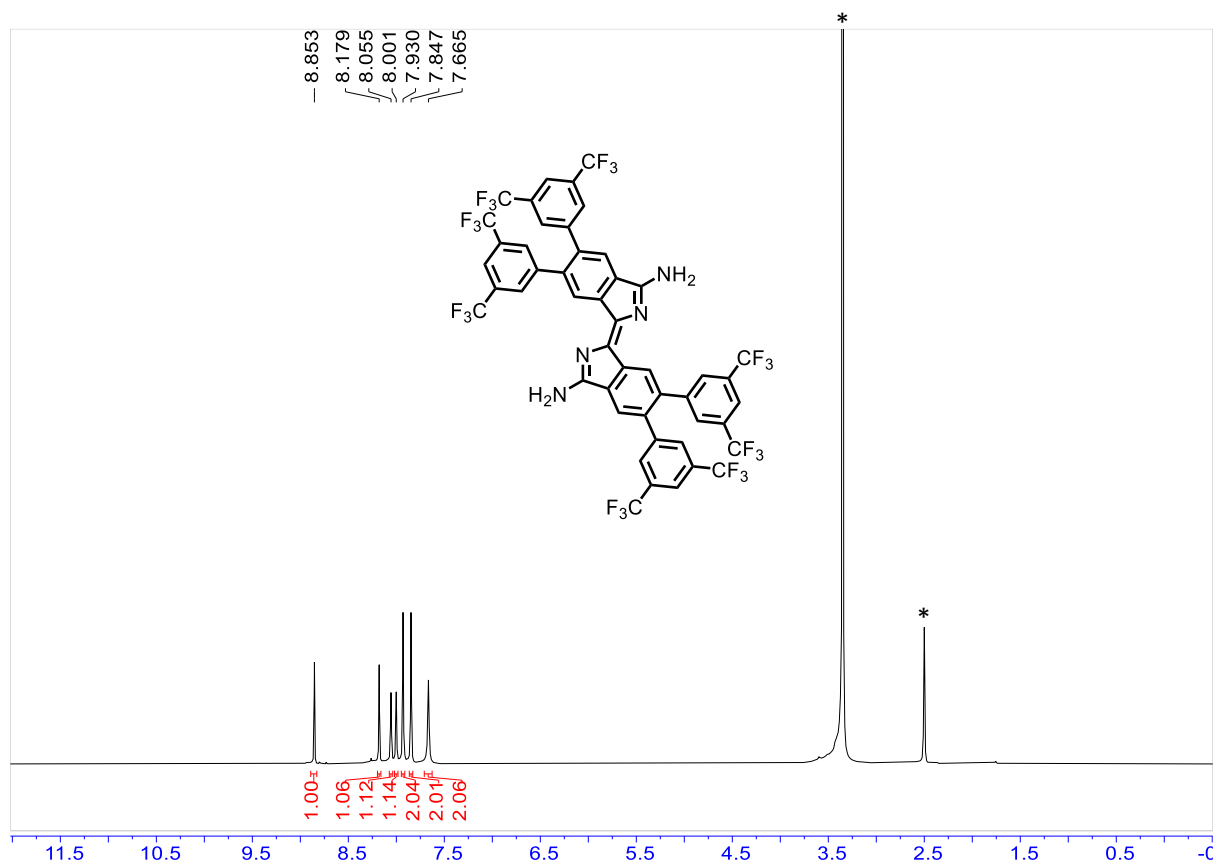


Figure S5. ^1H NMR spectrum of **4** in DMSO-d_6 (500 MHz). The signals due to the residual non-deuterated solvent and residual water are marked with an asterisk.

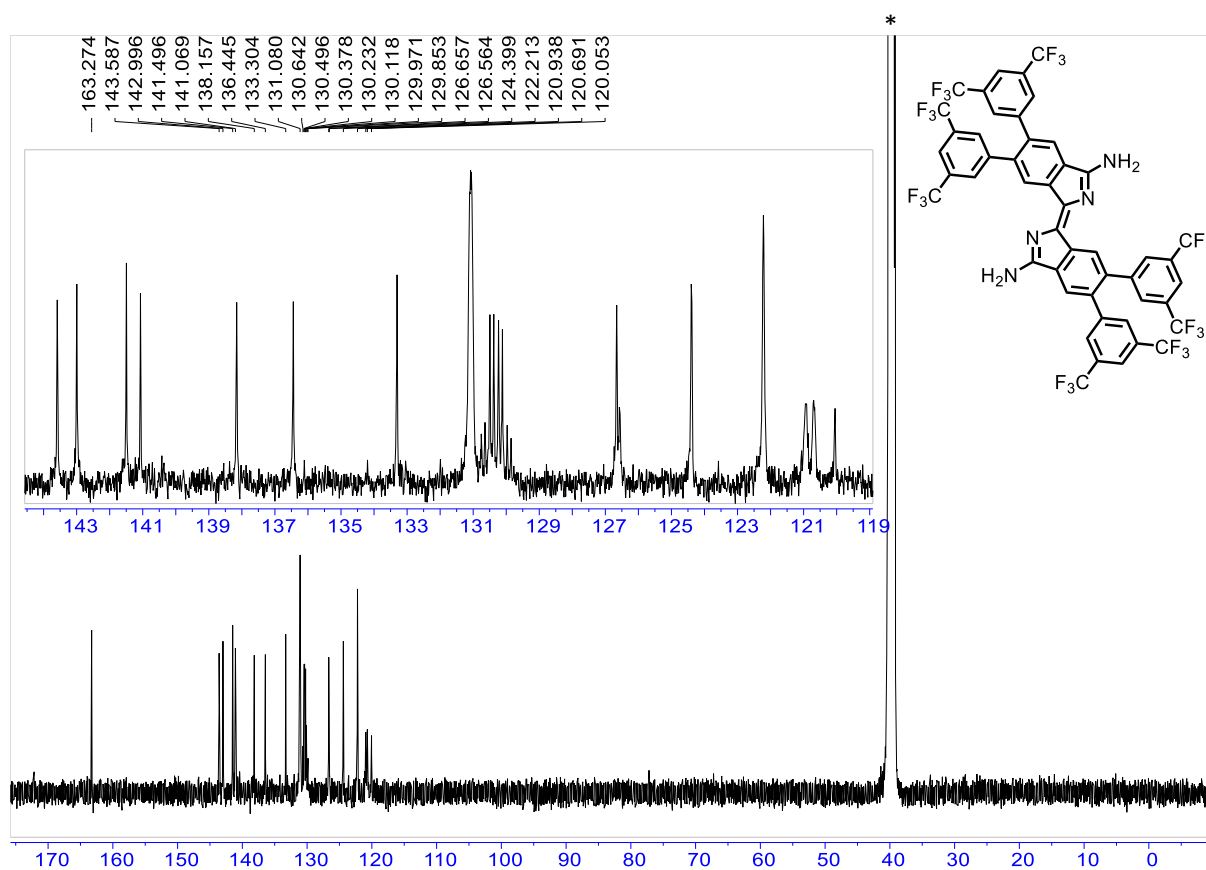


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4** in DMSO-d_6 (125.8 MHz). The signal due to the solvent is marked with an asterisk.

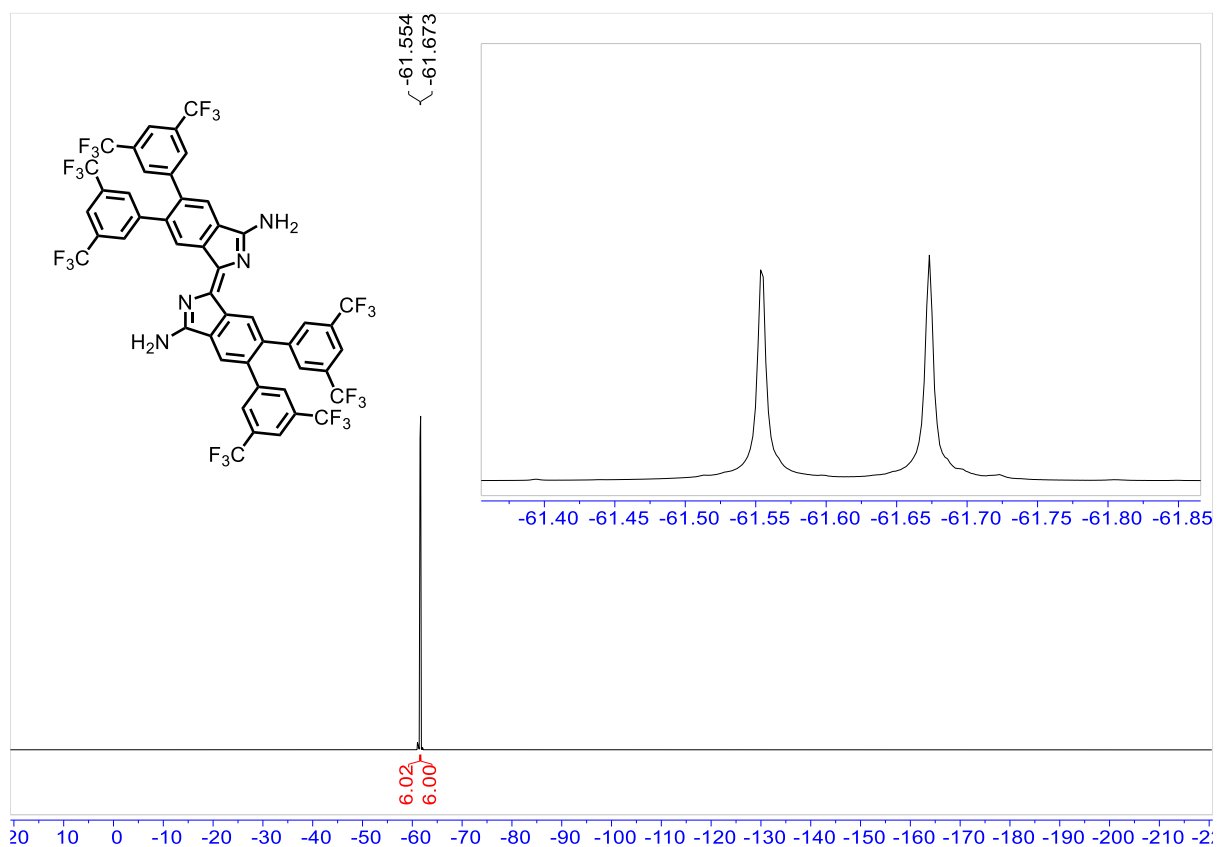


Figure S7. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **4** in DMSO-d_6 (470.4 MHz).

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CF3Ar-DABI

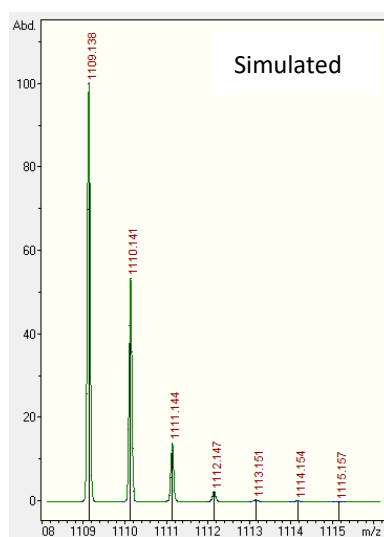
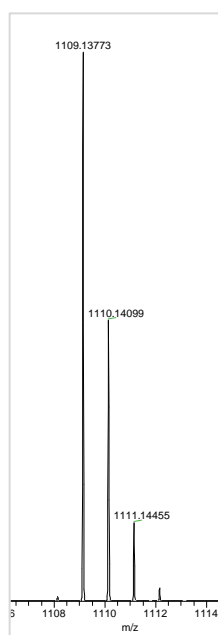
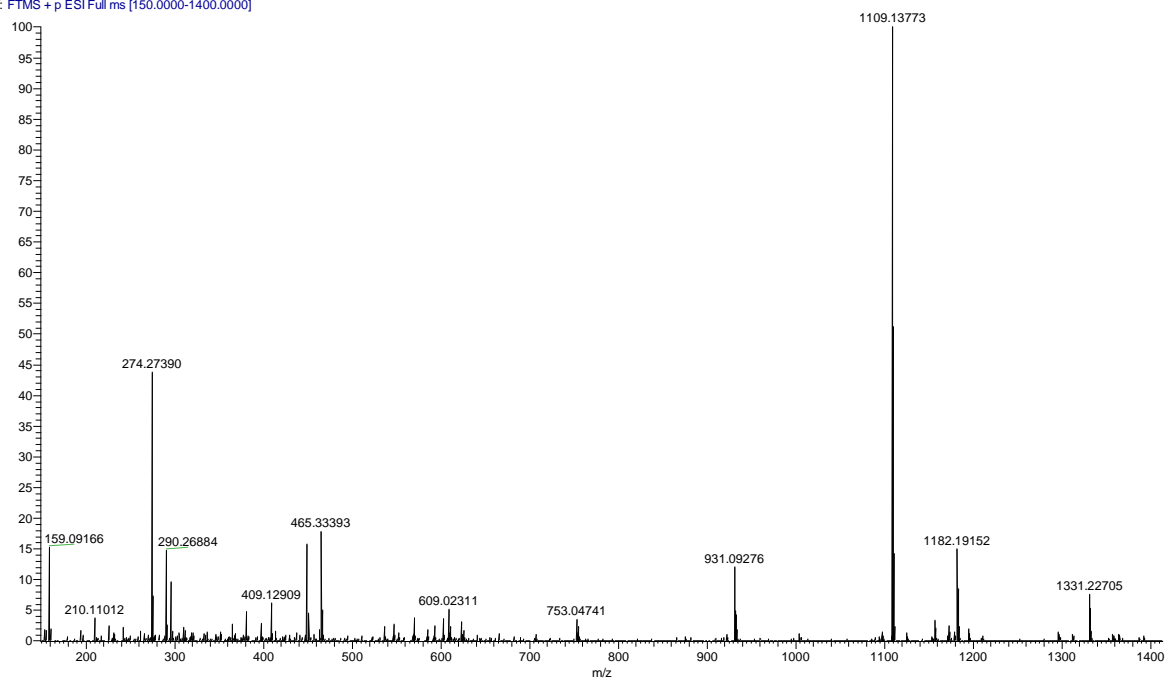
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T: FTMS + p ESI Full ms [150.0000-1400.0000]

Figure S8. ESI mass spectrum of **4**. The experimental and simulated isotopic patterns of the molecule ion signal are given in the lower part.

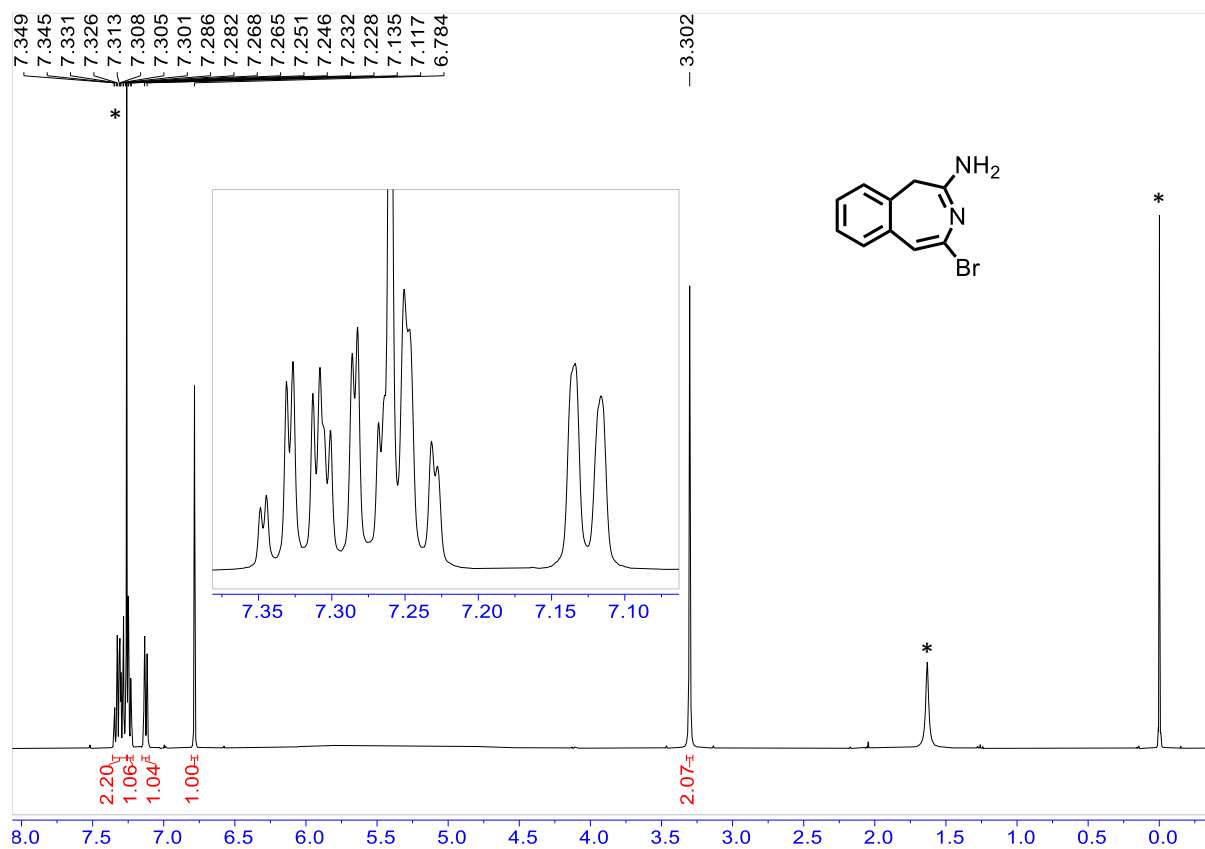


Figure S9. ^1H NMR spectrum of **7** in CDCl_3 (400 MHz). The signals due to the residual non-deuterated solvent, residual water, and SiMe_4 are marked with an asterisk.

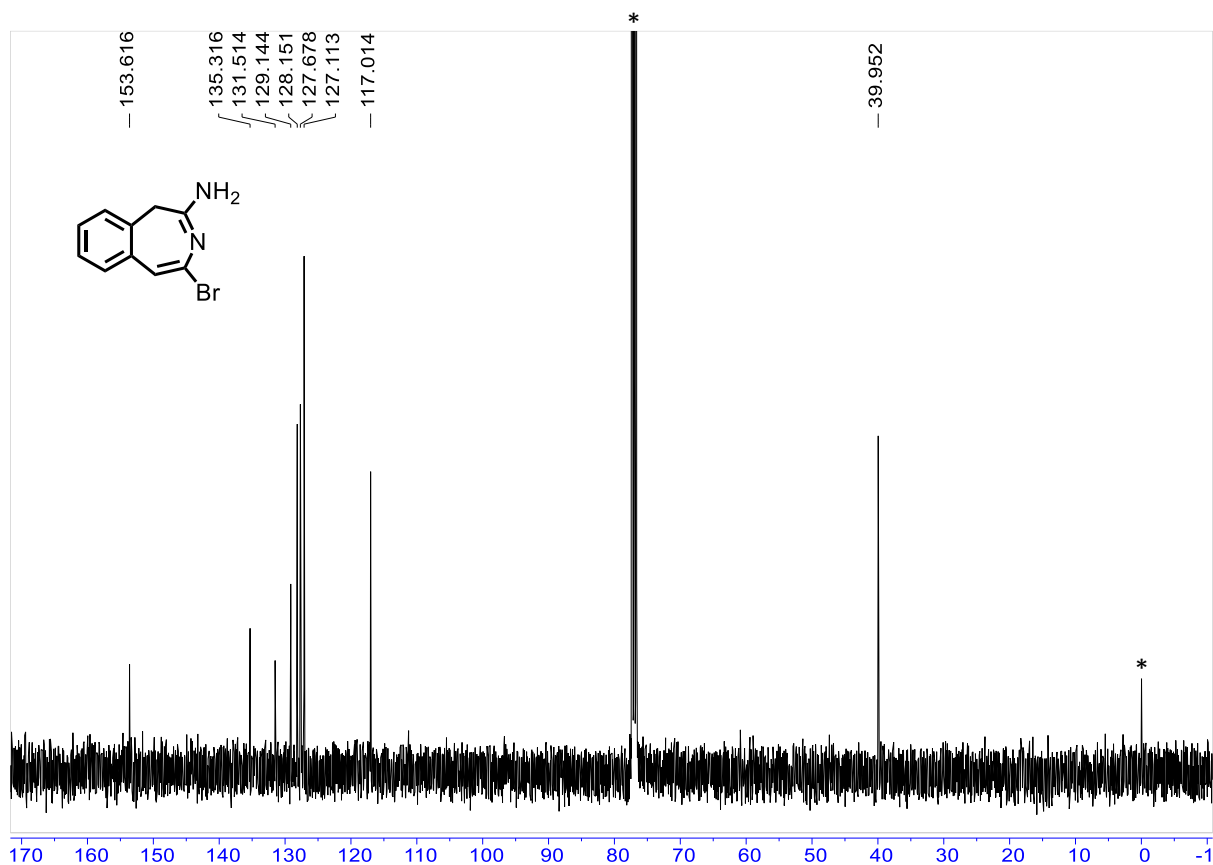


Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **7** in CDCl_3 (100.6 MHz). The signals due to the solvent and SiMe_4 are marked with an asterisk.

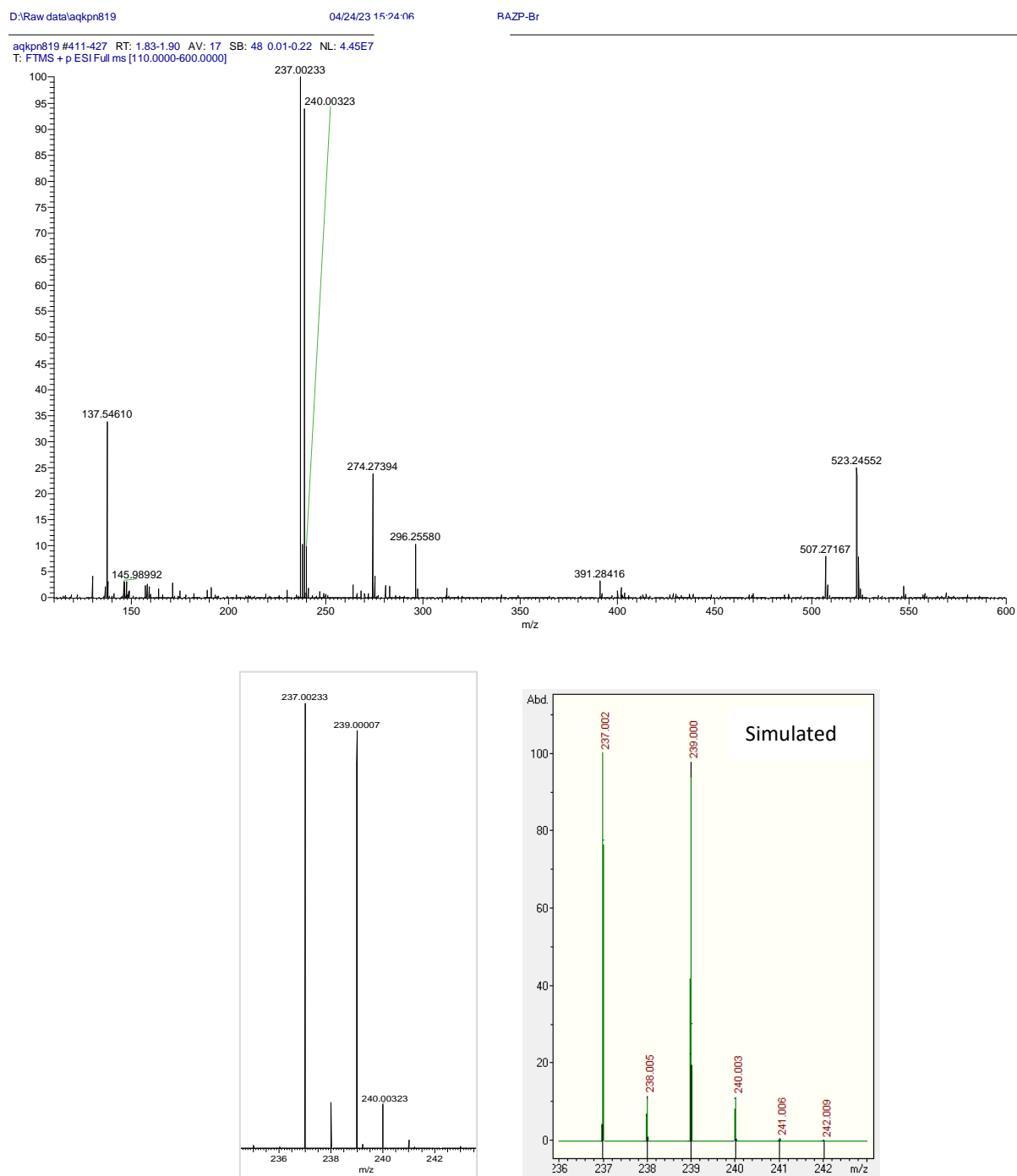


Figure S11. ESI mass spectrum of **7**. The experimental and simulated isotopic patterns of the molecule ion signal are given in the lower part.

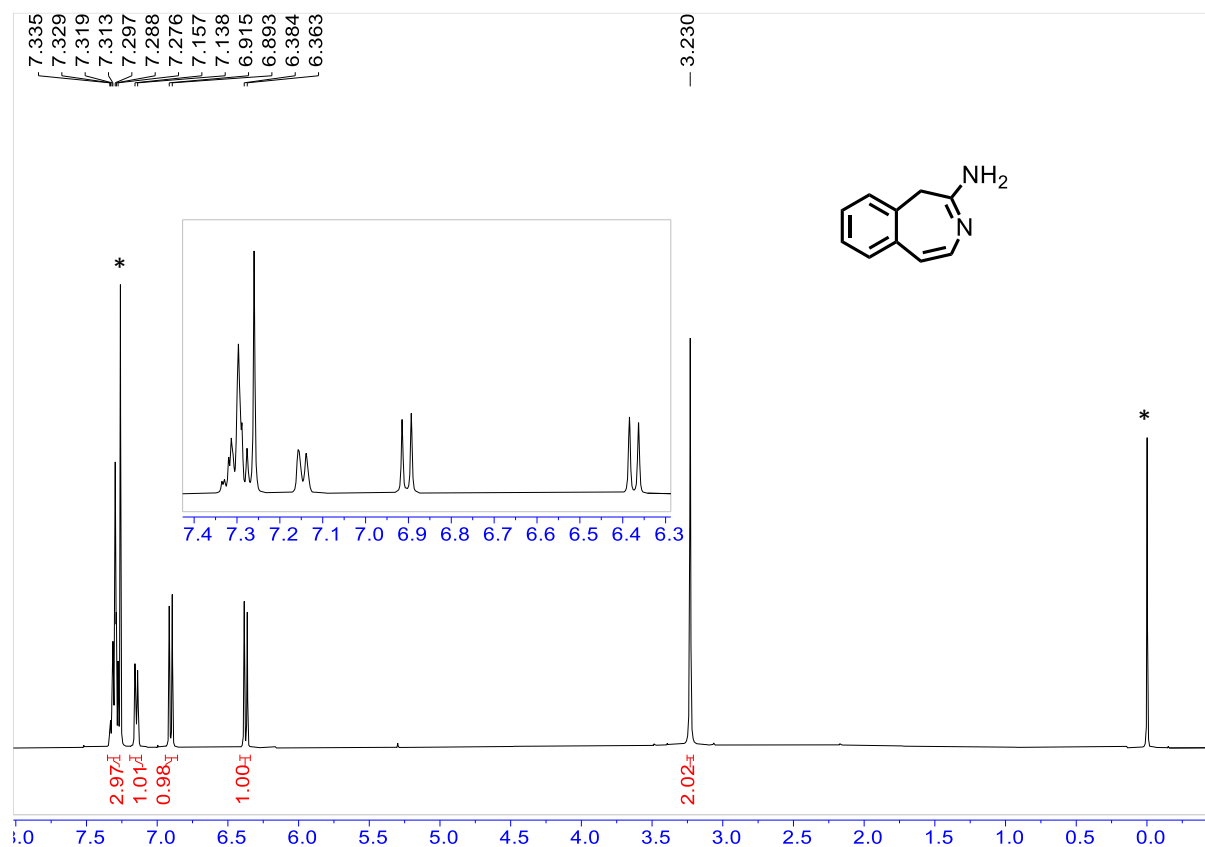


Figure S12. ^1H NMR spectrum of **5** in CDCl_3 (400 MHz). The signals due to the residual non-deuterated solvent and SiMe_4 are marked with an asterisk.

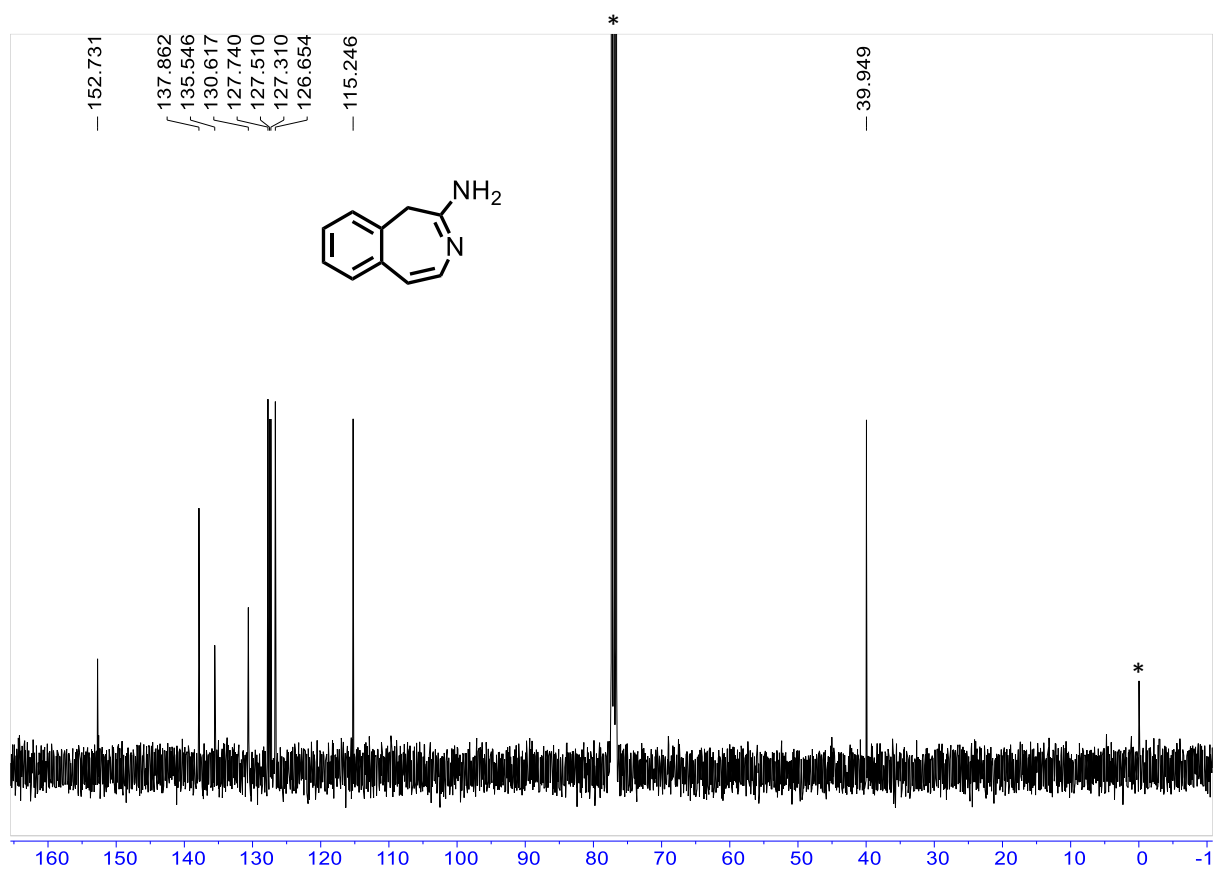


Figure S13. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5** in CDCl_3 (100.6 MHz). The signals due to the solvent and SiMe_4 are marked with an asterisk.

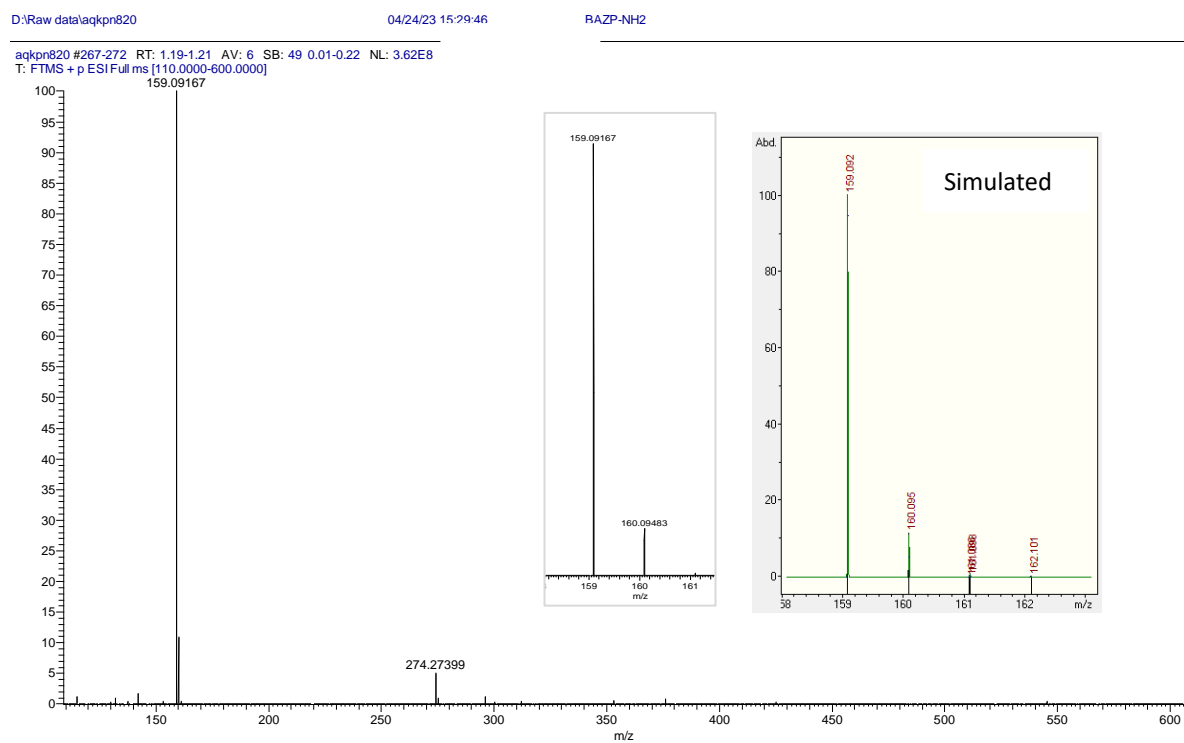


Figure S14. ESI mass spectrum of **5**. The experimental and simulated isotopic patterns of the molecule ion signal are given in the inset.

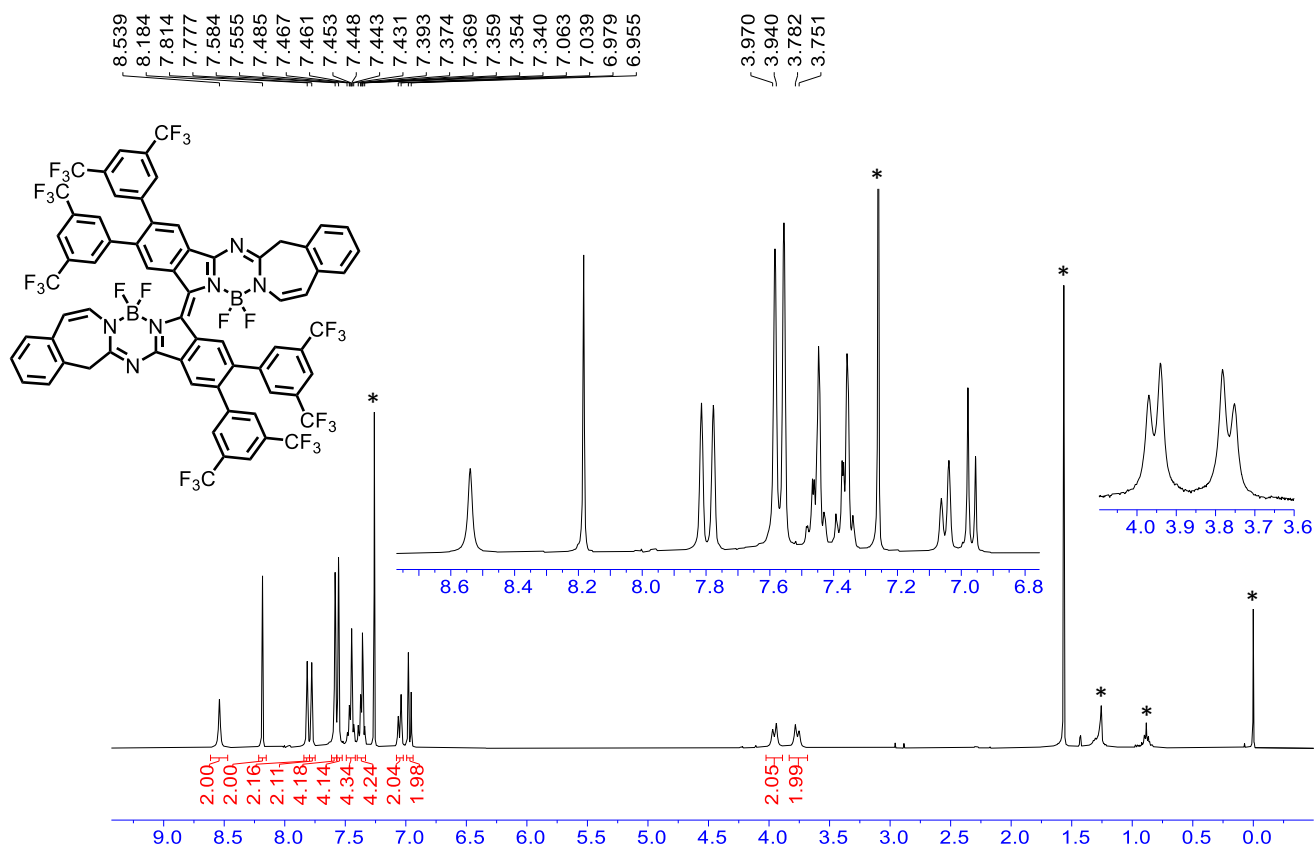


Figure S15. ^1H NMR spectrum of **9** in CDCl_3 (400 MHz). The signals due to the residual non-deuterated solvent, residual water, residual hexane used for chromatography, and SiMe_4 are marked with an asterisk.

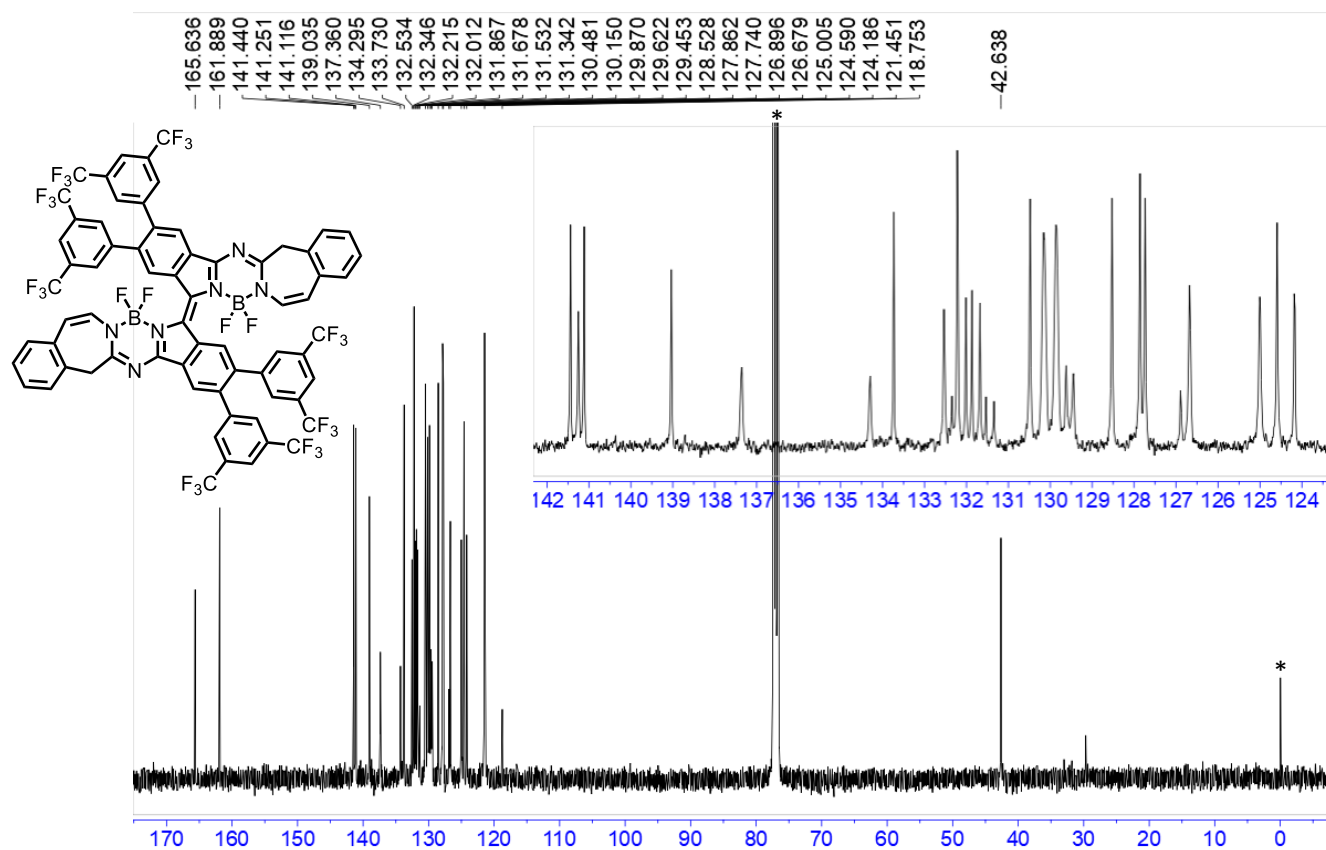


Figure S16. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9** in CDCl_3 (100.6 MHz). The signals due to the solvent and SiMe_4 are marked with an asterisk.

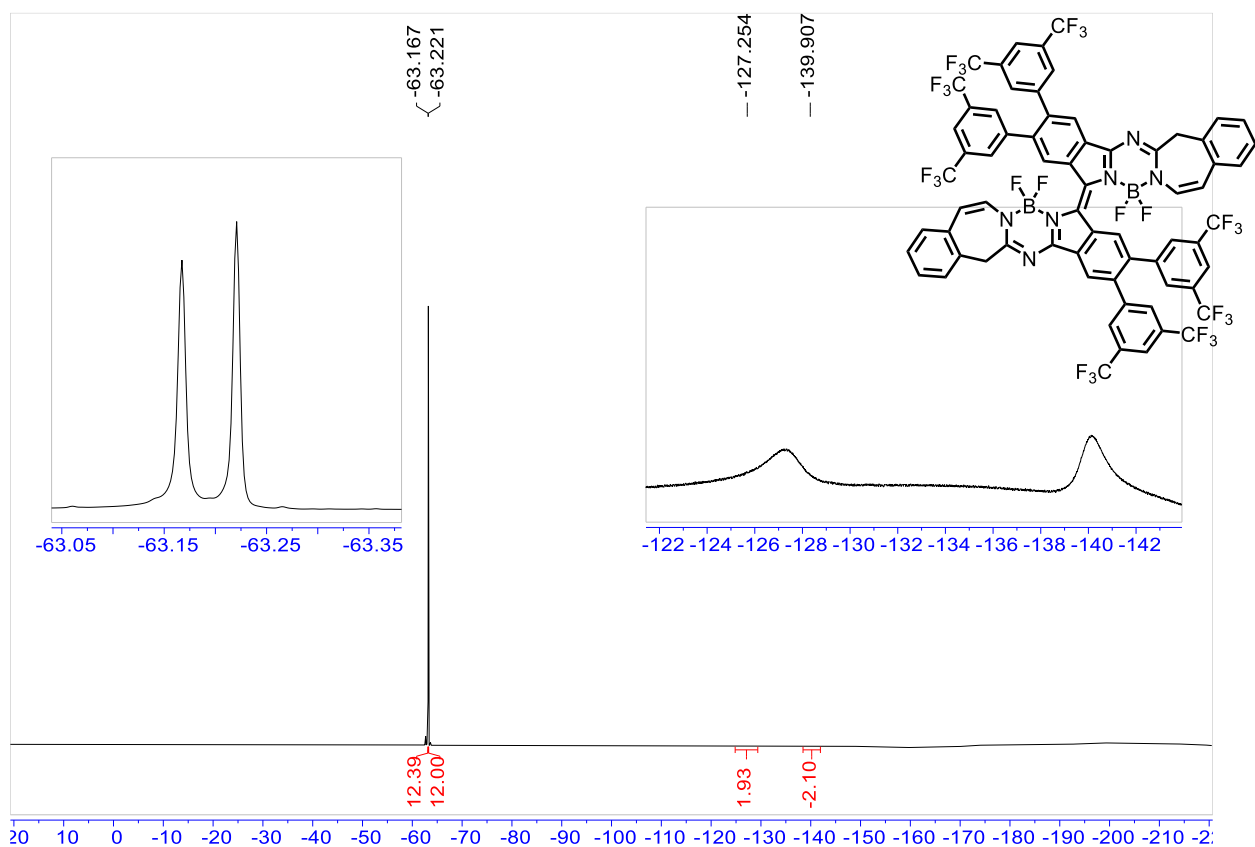


Figure S17. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **9** in CDCl_3 (470.4 MHz).

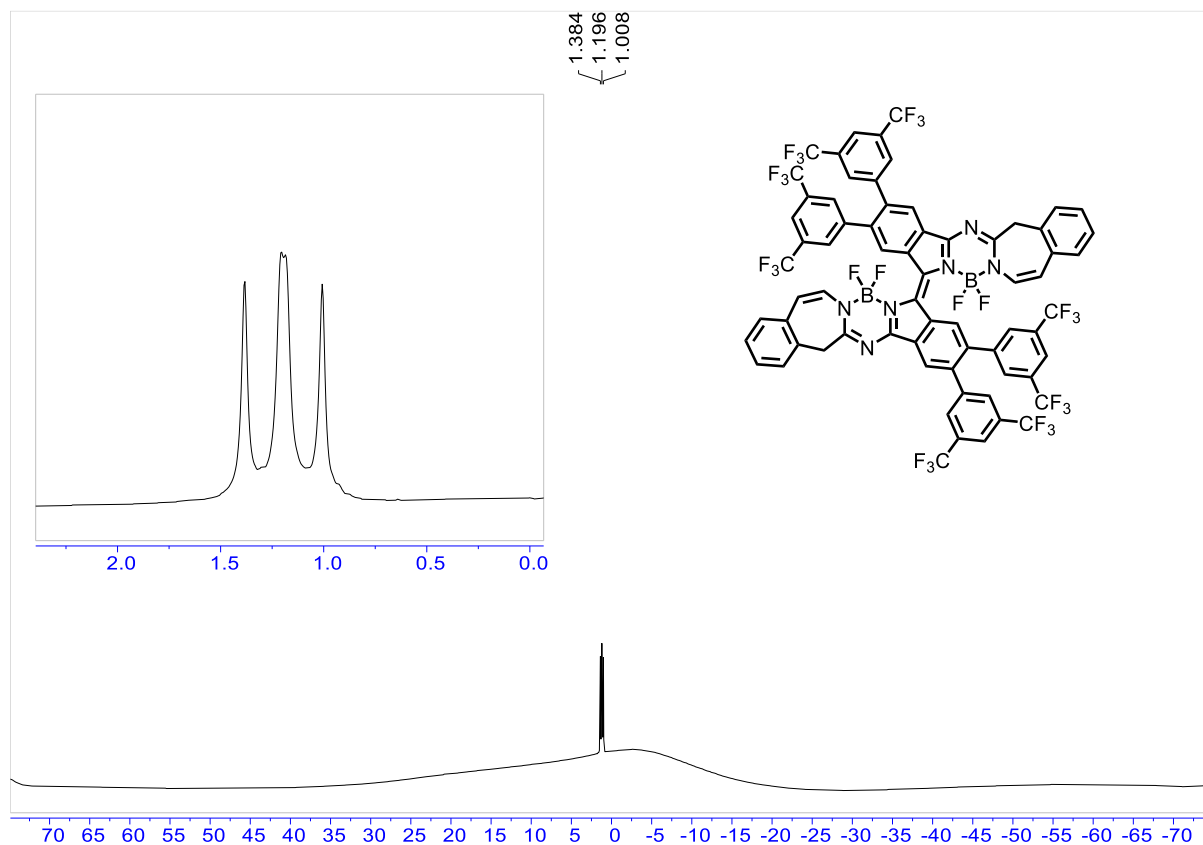


Figure S18. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **9** in CDCl_3 (128.4 MHz).

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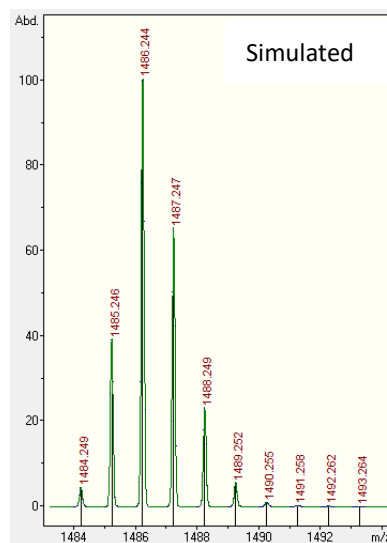
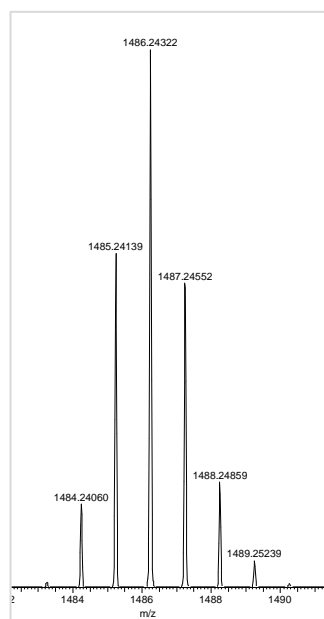
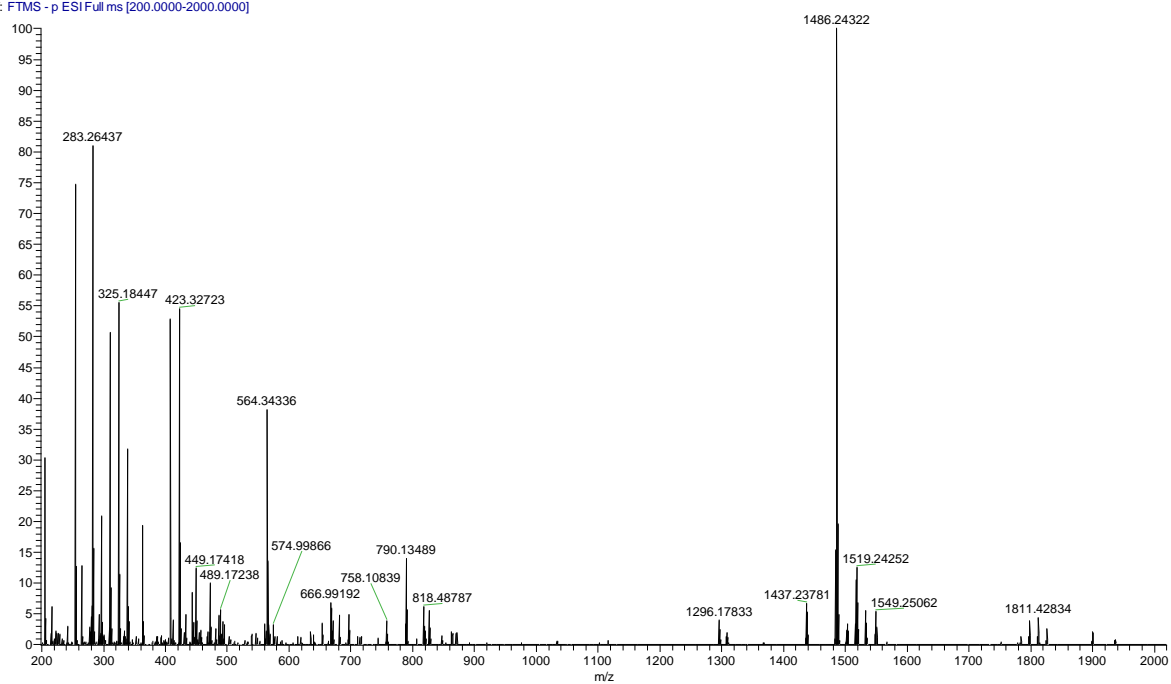
aqkpn750 #307-311 RT: 1.38-1.40 AV: 5 SB: 49 0.01-0.22 NL: 8.70E7
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Figure S19. ESI mass spectrum of **9**. The experimental and simulated isotopic patterns of the molecule ion signal are given in the lower part.

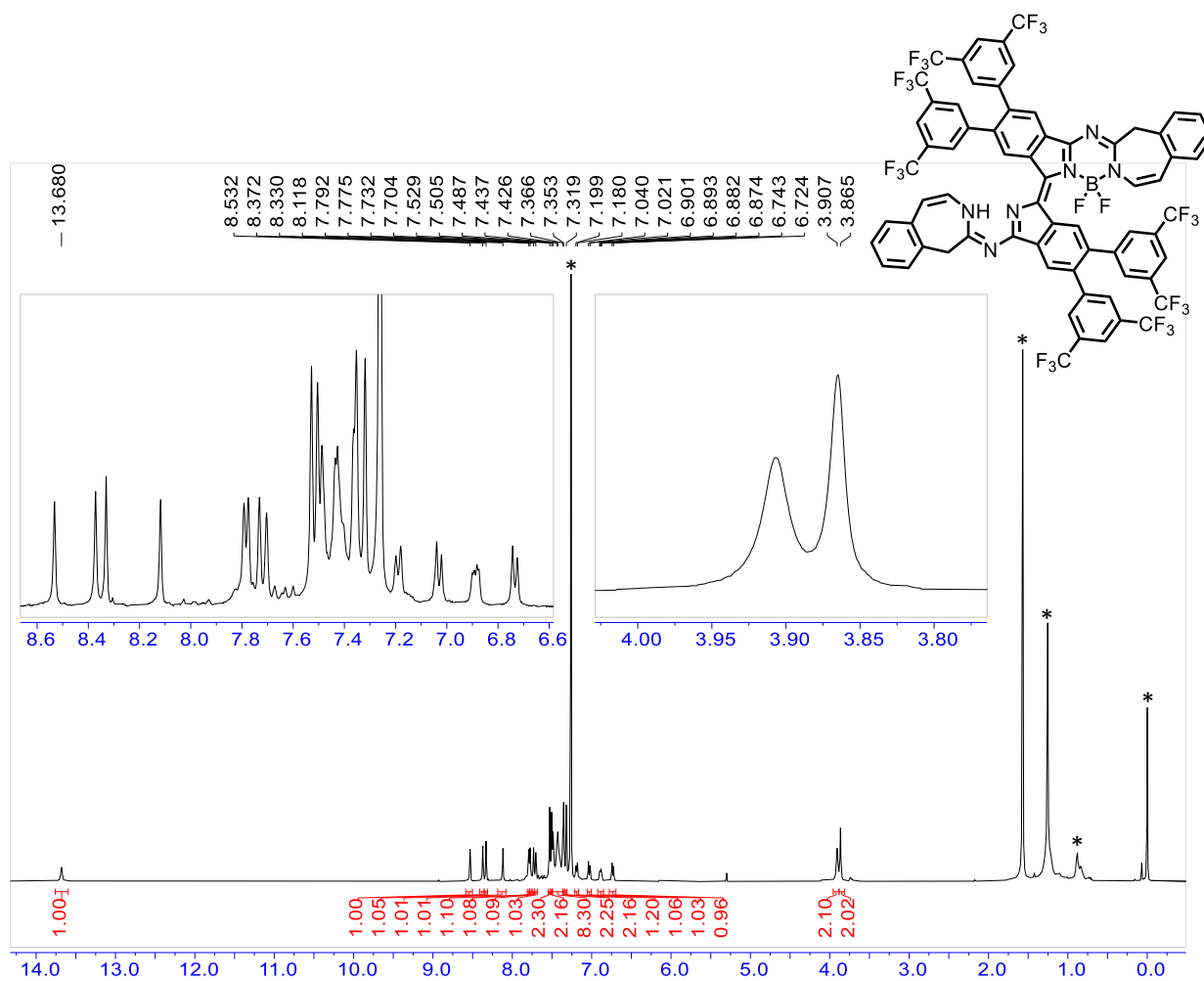


Figure S20. ^1H NMR spectrum of **11** in CDCl_3 (400 MHz). The signals due to the residual non-deuterated solvent, residual water, residual hexane used for chromatography, and SiMe_4 are marked with an asterisk.

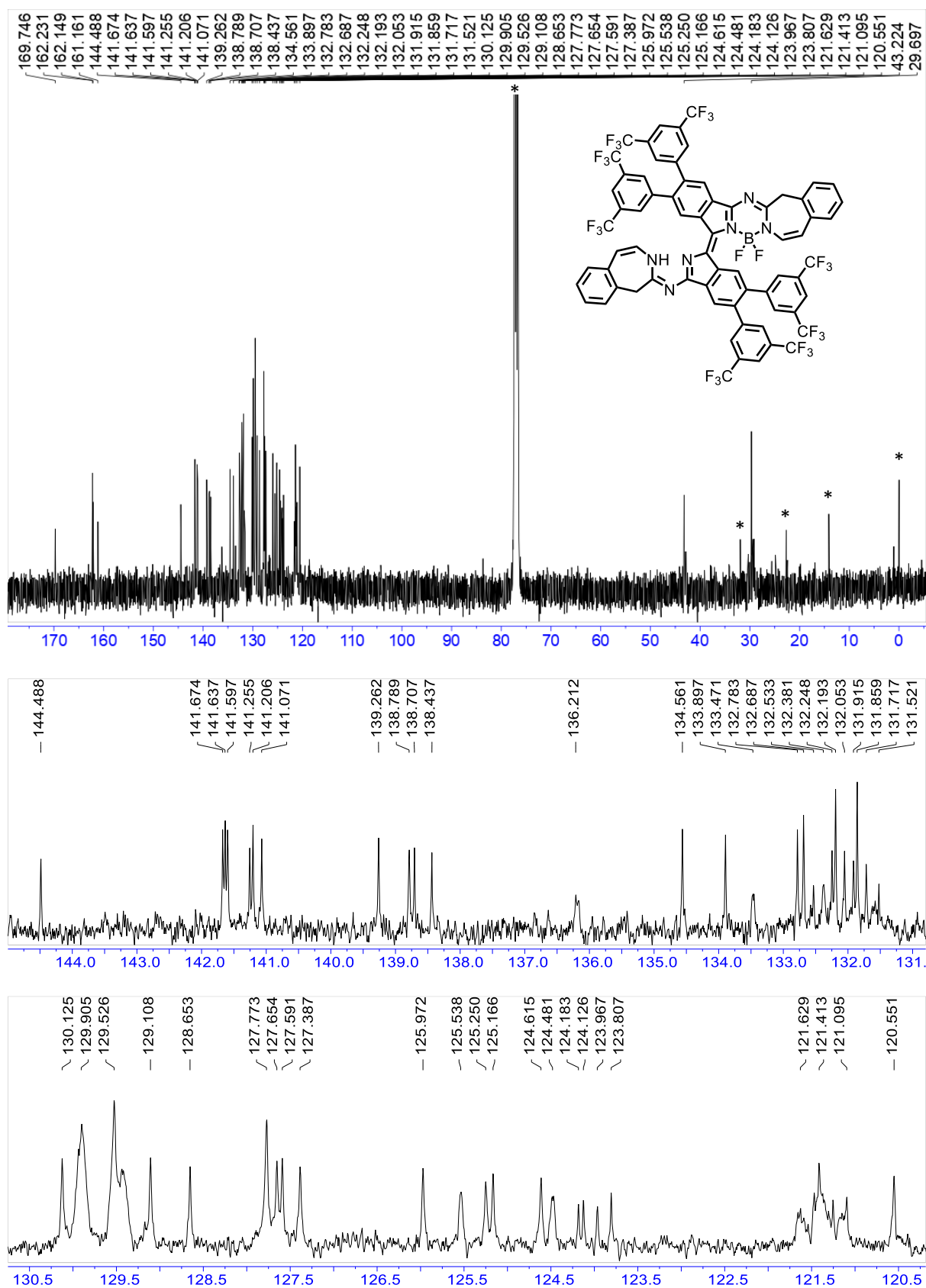


Figure S21. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **11** in CDCl_3 (100.6 MHz). The signals due to the solvent, residual hexane used for chromatography, and SiMe_4 are marked with an asterisk.

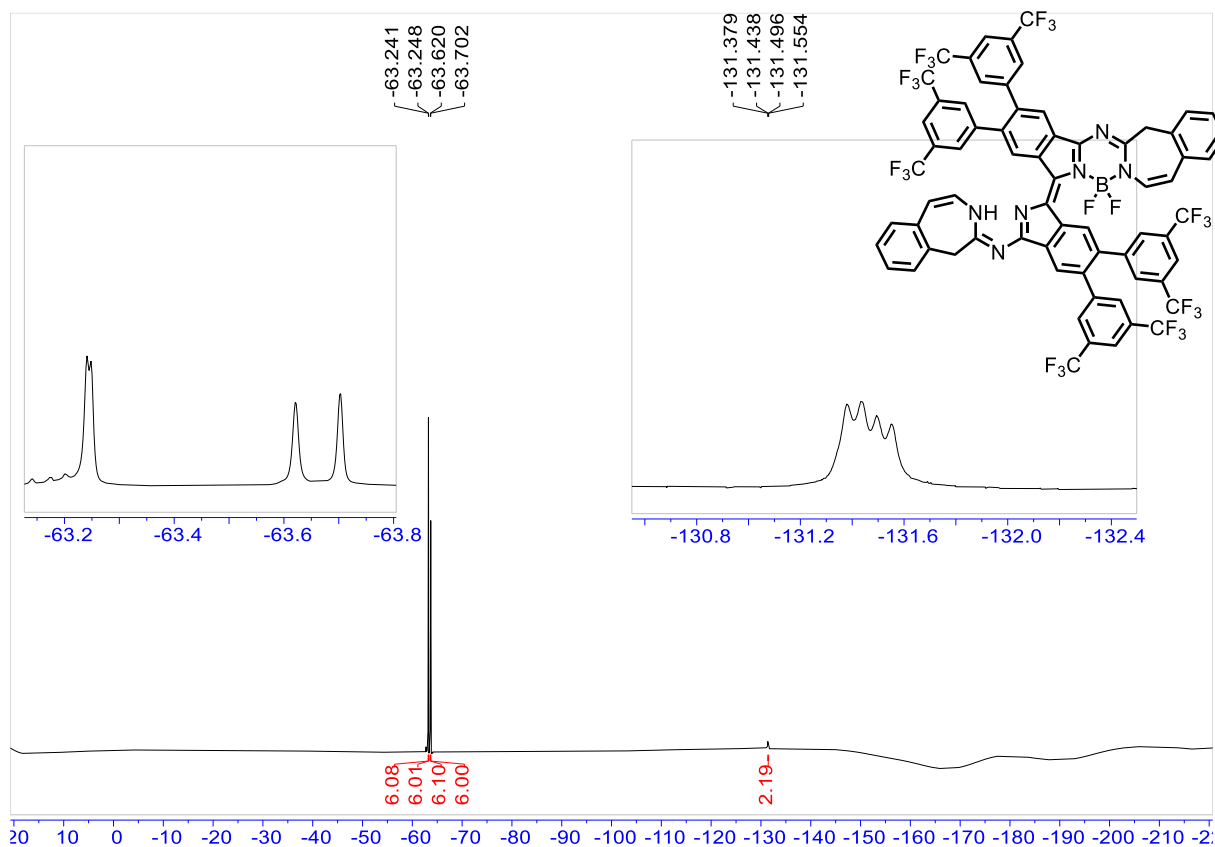


Figure S22. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **11** in CDCl_3 (470.4 MHz).

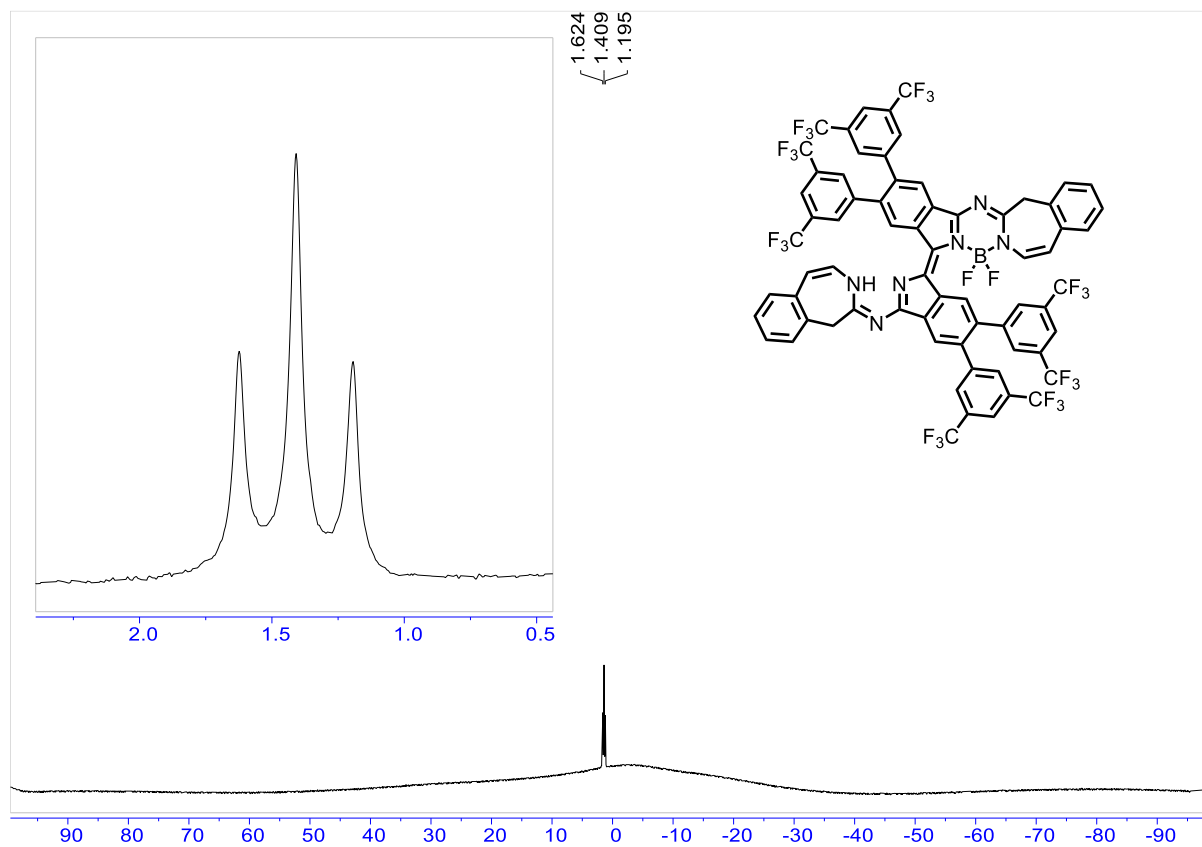


Figure S23. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **11** in CDCl_3 (128.4 MHz).

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Z1-272

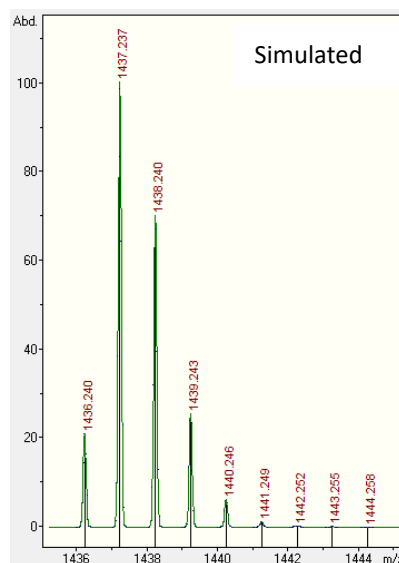
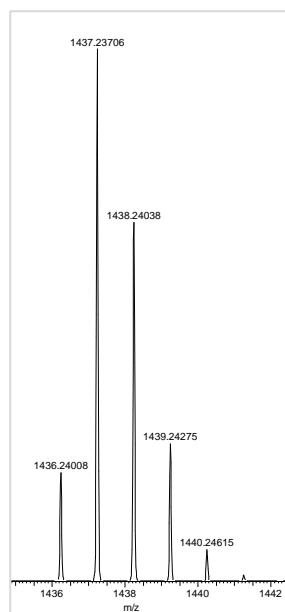
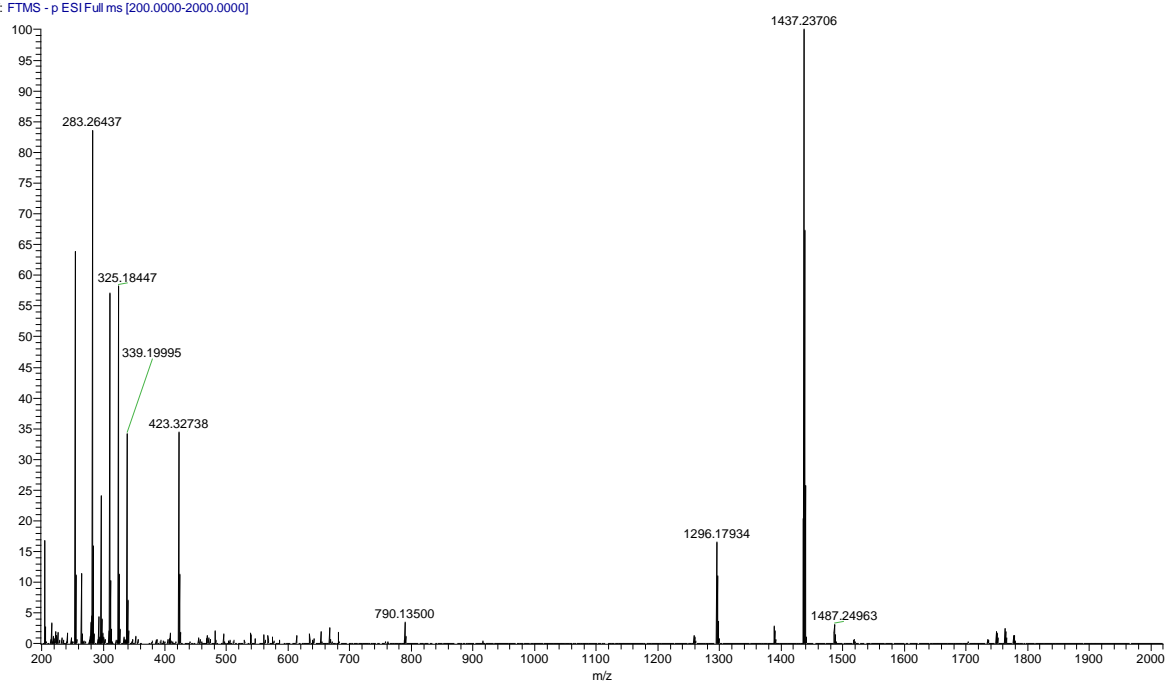
aqkpn751 #343-353 RT: 1.53-1.58 AV: 11 SB: 49 0.01-0.22 NL: 1.41E8
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Figure S24. ESI mass spectrum of **11**. The experimental and simulated isotopic patterns of the molecule ion signal are given in the lower part.